Abstract Submitted
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Broadband Phonon Scattering in PbTe-based Materials Driven Near the Peierls Phase Transition by Strain or Alloying[1] IVANA SAVIC, RONAN MURPHY, EAMONN MURRAY, STEPHEN FAHY, Tyndall National Institute, Cork, Ireland — Efficient thermoelectric energy conversion is highly desirable as 60% of the consumed energy is wasted as heat. Low lattice thermal conductivity is one of the key factors leading to high thermoelectric efficiency of a material [1]. However, the major obstacle in the design of such materials is the difficulty in efficiently scattering phonons across the frequency spectrum [2]. Using first principles calculations, we predict that driving PbTe materials close to a Peierls-like phase transition could be a powerful strategy to solve this problem. We illustrate this concept by applying tensile [001] strain to PbTe and its alloys with another rock-salt IV-VI material, PbSe; and by alloying PbTe with a IV-VI Peierls-distorted material, GeTe. This induces extremely soft optical modes, which increase acoustic-optical phonon coupling and decrease phonon lifetimes at all frequencies. We show that PbTe, Pb(Se,Te) and (Pb,Ge)Te alloys driven near the phase transition in the described manner could have the lattice thermal conductivity considerably lower than that of PbTe. The proposed concept may open new opportunities for the development of more efficient thermoelectric materials. [1] G. J. Snyder and E. S. Toberer, Nature Mater. 7, 105 (2008). [2] K. Biswas et al. Nature 489, 414 (2012).

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